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A Simplified, Semi-analytical Method to Handle Uncertainty in Long-term Containment in Geologic CO₂ Storage Sites

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Abstract

Carbon dioxide capture and storage (CCS) can contribute to stabilizing atmospheric content of carbon dioxide (CO₂) provided that it can deliver long-term storage containment. Satisfying this condition requires understanding and representing uncertainty in the underground. One of the major containment failures is due to opening of new or existing fractures or faults, or ingress through the cap rock barrier. In this study semi-analytical methods (e.g. first- and second-order reliability methods) are used to analyze and understand this isolated containment failure mode. This paper gives a brief introduction and description of the mathematics of the reliability method and how it can be applied to analyze the failure probability of CO₂ geologic storage using commercially available software.

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1. Introduction

Carbon dioxide capture and storage (CCS) can contribute to stabilizing atmospheric content of carbon dioxide (CO₂) provided that it can deliver long-term storage containment of the stored CO₂. Satisfying this condition requires understanding and representing uncertainty in the underground and in the long-term storage process itself, which may be influenced by a number of important and varied physical and chemical features, events and processes (FEPs). Data on the underground can be very sparse, and probabilities of failure of storage containment due to any one physical FEP at a single point in the system can be relatively low, yet there may be many such potential individual failures at a specific site. This combination may preclude using common Monte Carlo simulation techniques (and variants thereof) for risk assessment because of the slow convergence of models in which there are very many uncertain variables with relatively low probabilities. Such situations are well-known in the field of structural reliability analysis, in which semi-analytical methods (e.g. the first- and second-order reliability methods,

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FORM and SORM, respectively) are preferred to analyze and understand overall system performance where failure tolerance is small.

Uncertainty in the physical and chemical parameters in the subsurface in general is ubiquitous, and CO₂ geologic storage is no exception. This is manifested primarily in the basic heterogeneity of aquifer formations and the uncertainty related to the chemical and physical interaction of injected CO₂, subsurface mineral compounds and the dissolved compounds in aquifer brine. Furthermore, there is a great deal of uncertainty regarding the leaking feature dimensions, e.g. subsurface leakage through faults and subsequent concentration of CO₂, leaking rate and duration. These parameters vary largely from one site to another and may also exhibit great spatial variability within the same site. In many applications, consideration of the uncertainty constitutes an integral part of the modelling process. During the storage of CO₂ in geological formations there are different sources of uncertainty that the geoscientist has to account for. These uncertainties may arise from using a simplistic relationship to describe the actual behaviour of a physical system or simply due to lack of knowledge of the system. They may arise also during data collection, recording, and analysis. In some cases data are collected in the field, and statistical estimators (mean and higher order moments) are obtained, and a probability density function (PDF) is chosen to represent the distribution of each input probabilistic variable. Since collected data are usually sparse and noisy, those PDFs are bound to be biased [1]. Another type of uncertainty is that resulting from the inherent randomness of the medium variables under consideration. This is quite evident in the aquifer formations, for which properties such as permeability can span many orders of magnitude at the same site [2]; [3]. This type of uncertainty is irreducible, and is often referred to as the *inherent, intrinsic, or physical uncertainty* [4]; [1]. Although the current research focuses on addressing the physical uncertainty, the approach is equally applicable to other types of uncertainty with the necessary modifications of the formulation.

The reliability methods have been widely applied in structural reliability analyses [4, 5] and have been tested in studying the uncertainty in groundwater contaminant transport [6]. This paper illustrates applying semi-analytical reliability methods to a CO₂ storage site to analyze its long-term containment using the general purpose probability analysis (PROBAN) software package that is designed for sophisticated probabilistic analysis [7]. Many of the sources of possible containment failure are due to the storage of CO₂ in porous and permeable reservoir rock at pressures higher than that in the surrounding formation, which can lead to opening of new or existing fractures or faults, or ingress through the cap rock barrier due to exceedance of capillary entry pressure. A different type of failure is damage or degradation of the cement sheath around wellbores or cement plugs inside and subsequent corrosive breach of casing, leading to leakage along or inside abandoned wellbores, especially where knowledge about their existence, status, number and location is low. And perhaps the most intuitive low-probability event is natural seismic and tectonic activity which can cause containment failure due to faulting, fracturing of the underground and possibly destruction of wellbores. All these problems can be modelled in the framework of the method of reliability analysis. However, the current study demonstrates the method of reliability analysis on one of the problems, namely the leakage along a single fault. The reliability method is described in Section 2. Some applications of the reliability method are given in Section 3 with details of its application in the case of CO₂ geological storage as presented in Section 4. The results are presented in Section 5 and finally the discussions and conclusions are highlighted in Section 6.

2. Description of the reliability methods

The first- and second-order reliability methods (FORM and SORM, respectively) were originally developed in the past 25-30 years to assess the safety of structural components and structural systems and are now widely used in the study of structural reliability problems. This section presents a brief review of the method of reliability analysis to the extent necessary to understand the subsequent formulation of the problems. A full account of the reliability methods development and evolution can be found in [5], [8], [4], and [9].

In component reliability formulation the uncertain parameters involved in the problem describing the component of interest are represented by a set of n -probabilistic variables, $X = (X_1, X_2, \dots, X_n)$. These are termed the *basic probabilistic variables* or *uncertain variables*. The *limit-state function* (also termed *performance function*) is a scalar

function of the input probabilistic variables, $g(\mathbf{X}): \mathbf{IR}^n \rightarrow \mathbf{IR}$. When the vector of probabilistic variables \mathbf{X} has the realization $\mathbf{x}=(x_1, x_2, \dots, x_n)$, then the value $g(x_1, x_2, \dots, x_n)$ determines the *state* of the component for that particular realization.

The g -function is formulated with the convention that if $g(x_1, x_2, \dots, x_n) > 0$, the component has *survived*, whereas if $g(x_1, x_2, \dots, x_n) < 0$, then the component has *failed*. Consequently, the space \mathbf{IR}^n of the physical probabilistic variables is divided into two domains:

$$S = \{x; g(x) > 0\} \quad \text{denotes } \textit{safe} \text{ domain, and} \quad (1)$$

$$F = \{x; g(x) < 0\} \quad \text{denotes } \textit{failure} \text{ domain} \quad (2)$$

The n -dimensional hypersurface $\{x; g(x)=0\}$ is the limiting condition between failure and survival, and is termed the *limit-state surface*.

Note that the term *component* in this context means that there is a single mode of failure. To state it simply, the component of interest would either fail or survive. This is different from the *system reliability* formulation, however, where the system has more than one failure mode and some degree of component redundancy. In *component reliability* problems, situations with a single failure mode are analyzed. In *system reliability* problems, however, we consider the problem of evaluating the reliability of a system where the state is described by more than one limit-state function. This is important in exposure assessment situations where the interest is for example on more than one abandoned well, or when assessing the performance of a storage site based on the success to meet the containment at a few points (e.g. wells and/or fractures) in the storage formation. In this case, the state of the system is described by the states of its components.

The probability of failure is given by the n -fold integral,

$$P_F = P[g(X) \leq 0] = \int_{g(X) \leq 0} f_X(x) dx \quad (3)$$

where $f_X(x)$ is the joint probability density function of X and the integration is carried out over the failure domain [6]. In other words, the failure probability is the probability of being in the domain of the n -dimensional space bounded by $g(\mathbf{X}) \leq 0$. A variety of factors complicate the direct estimation of this n -fold integral and prevent the use of the standard methods of integration and thus the primary objective of the reliability methods is to overcome the difficulties and to evaluate the multidimensional integral in (3) [6]. FORM and SORM are analytical schemes used to approximate the probability integral when the basic variables have strictly increasing continuous joint cumulative distribution functions.

FORM and SORM consist of a number of steps [10]: (1) transformation of the basic variables, \mathbf{X} , into the standardized and uncorrelated normal variates, \mathbf{U} (2) determination of the most likely failure point in the standard space, (3) approximation of the limit-state surface in the standard space at the design point, and (4) computation of the probability of failure in accordance with the approximation surface selected in step (3).

Additional benefits of the first- and second-order reliability methods are that the user is provided with measures of sensitivity of the failure probability with respect to the basic probabilistic variables. Moreover, valuable information to the parametric sensitivity factors is provided by the uncertainty *importance factors* of the failure probability [11]. Importance factors allow for the identification of the probabilistic variables which have the least impact on the final reliability outcome and are very useful in reducing the number of basic probabilistic variables in large size reliability models and for focused gathering of more information to reduce uncertainty associated to these variables. All these issues are handled by the PROBAN software package that comes equipped with a distribution library that contains more than twenty probability distributions.

3. Selected example applications of reliability methods

The classic example of application of the reliability method is in structural reliability analysis with the limit-state function definition addressing the “load-resistance” problem [7]. In such a problem, the resistance of a given structural component, R , is assumed probabilistic, for example due to material imperfections. The load applied on the structural component, L , is also assumed probabilistic. Wind and earthquake loads are examples of such probabilistic loading. Now the limit-state function is typically formulated as follows:

$$g(R, L) = R - L \quad (4)$$

Therefore, realizations that cause the g -function to be negative indicate that the structural component has *failed* to withstand the applied load (Equation 2). On the other hand, realizations resulting in positive values of the g -function indicate a condition where the structure has *survived* in withstanding the applied probabilistic load (Equation 1).

Another application of the first- and second-order reliability methods is the study of the uncertainty in groundwater, contaminant transport [6]. One of the problems of interest in this context was to study the probability that the concentration of a given contaminant leaking continuously from a source exceeds a pre-determined target level at a down gradient water supply well during the simulation time of interest. In one of the cases studied, they looked at the normalized target concentration at the receptor well, $(C(X)/C_0)$, where C_0 is the source concentration and $C(X)$ is the simulated concentration when parameter uncertainty is taken into account. Hence the limit-state function was formulated as follows:

$$G(X) = (C/C_0)_{target} - C(X)/C_0 \quad (5)$$

where $(C/C_0)_{target}$ is the pre-specified normalized target concentration at the well.

Component failure occurs when $g(\mathbf{x})$ (for a given realization \mathbf{x} , of the probabilistic variables) is less than zero; that is, when the normalized target concentration at the receptor well is exceeded. Equations (4) and (5) are examples of *component reliability* problems, situations where a single failure mode are analyzed. In the groundwater context, examples include failure to meet regulatory concentration levels at a single receptor well in the vicinity of a hazardous waste site, or failure to meet the target remediation cleanup levels for a specific well at a contaminated site. In *system reliability* problems, however, we consider the problem of evaluating the reliability of a system where the state is described by more than one limit-state function. This is important in exposure assessment situations where the interest is for example on more than one abandoned well, or when assessing the performance of a storage site based on the success to maintain containment at a few points (e.g. wells and/or fractures) in the storage formation. The limit-state function for the system reliability can be formulated in similar way which will not be discussed in this paper.

4. An example application in CO₂ geologic storage

The reliability method is demonstrated here on the probability of leakage from a hypothetical fault shown in figure 1. The primary general question is what is the probability of CO₂ leakage rate from a storage site will exceed a threshold level; Ancillary questions are related to the sensitivity of this probability to the input probabilistic variables.

The fracture flow modelling approach pursued here follows the strategy in [12] which scales up properties of fracture flow zones from explicitly described permeability features to equivalent large-block permeabilities in finite-difference flow simulators. For a rectangular region of physical dimensions L_x , L_y and L_z , with a pressure difference Δp imposed in the z direction and the z - z component of permeability (k_{zz}), the flow rate along the z -direction is given by

$$Q_z = \frac{k_{zz} k_{rg} L_x L_y \Delta p}{\mu_\alpha L_z} \quad (6)$$

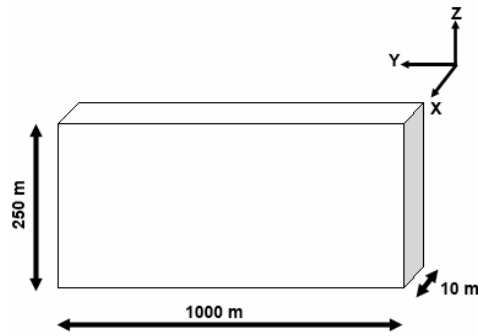


Figure 1: Fault block model.

where Q_z is the total flow rate through the fault plane, k_{zz} is the permeability parallel to the fault plane and is considered here isotropic. L_x , L_y , and L_z are the lengths of the fault along the x -, y - and z - directions, respectively (Figure 1). μ_a is the viscosity of the fluid (CO_2). Mobility of the CO_2 is a function of the relative permeability (k_{rg}) and the viscosity (μ_a) and is defined as k_{rg}/μ_a . Here the relative permeability of CO_2 is taken 1 (fully saturated condition). The simplifying assumptions are that the pressure gradient lies entirely in the plane of the fracture, resulting in a unidirectional (vertical) flow through the system and that the fault system is parallel to the principal directions of permeability thus, the cross terms of permeability are assumed small and thus neglected. The limit-state function is defined as:

$$g(x) = Q_{Th} - Q_{Cal} \quad (7)$$

Equation (6) is used to calculate the leakage rates along a fault using a range of intrinsic permeability values given in Table 1. Later the limit-state function given in Eq. (7) is adopted to solve the reliability problem by setting threshold values, varying the term Q_{Th} in Eq. (7) each time. *Component failure* occurs when $g(x)$ (for a given realization x , of the probabilistic variables) is less than zero; that is, when the calculated leakage rate (Q_{Cal}) is greater than the predefined threshold leakage rate (Q_{Th}). Natural analogues such as CO_2 flux rates from faults can be useful for estimating CO_2 leakage rates and constrain potential leakage rates and durations for the risk and uncertainty analysis of geological storage sites [13]. A range of flow rates of 0.001 - 60 tonnes/yr are observed from natural analogues and thus may be appropriate to apply for fault leakage. For a fault with $10 \times 1000 \text{ m}^2$ area coverage (width \times strike-length) and assuming a maximum of 6 tonnes/yr/ m^2 CO_2 flux rate its leakage rate would be 6×10^4 tonnes/yr, or 165 tonnes/day. This approach is used to define the threshold leakage rates (Q_{Th}) in Eq. (7).

Table 1: Deterministic and probabilistic input parameters used for the calculation of CO_2 leakage rate from a fault

Variables	units	Values
¹ CO_2 viscosity (μ_a)	Pa.s	3.95×10^{-5}
¹ Relative permeability (k_{rg})	----	1.0
² Leaky fault permeability (k_{zz})	mD	LN(0.01,002), (0.1, 0.02), (1,0.2) (10,2.0) and (100,20)
² Pressure difference along the fault (Δp)	MPa	N(4,0.8)
² Fault vertical length(height) (L_z)	m	N(250,50)
² Fault length (L_x)	m	N(10,2)
² Leaky fault width (L_y)	m	N(1000,200)

¹Deterministic, ²Probabilistic variables, N: Normal(mean, std. dev.), LN: Lognormal (variable) 1milliDarcy= $1.0 \times 10^{-15} \text{ m}^2$

The parameter uncertainty at the leaking fault located within the CO₂ plume area was studied in this case, considering the permeability of the fault, the dimensions of the fault along with the pressure difference in the aquifer as probabilistic variables and the relative permeability as well as the viscosity of the CO₂ as deterministic variables (Table 1). Since many geoscience-related variables have either normal or log-normal distributions, their means and standard deviations are used to represent them. Other main assumptions include: (1) the fault has known dimensions and intersects the storage formation including the cap rock (2) Constant density and viscosity of CO₂ (3) Pores in the fault zone are fully saturated by the CO₂, and (4) there exists after the start of injection a pressure gradient in the fault plane that drives CO₂ upward.

5. Results

In this assessment the analysis is carried out for a set of threshold leakage rates at a fault where its leakage rate is calculated at various intrinsic permeability values (Table 1). The reliability problem is solved a number of times, varying the thresholds that appear in Equation (7) at each time. Note that the probability distribution of the failure event under consideration can be obtained by varying the threshold values and using the parametric sensitivity results with respect to limit-state function parameters. This gives a more flexible way of assessing the risk of CO₂ leakage at any selected threshold values.

Figure 2 shows that results from FORM and SORM gave essentially identical results, which is not surprising given the simple linear problem analyzed. In general the failure probability decreases as the threshold leakage increases for a given permeability value except for the very high ($K=100$ and 10 mDarcy) cases which failed for all threshold limits. Also the probability of failure decreases as the intrinsic permeability of the fault decreases. For a given fault permeability the probability of failure decreases as the leakage thresholds increase. For lower fault permeability (e.g. $K \leq 1$ mDarcy) the probability of failure is reasonably low for a wide range of threshold values.

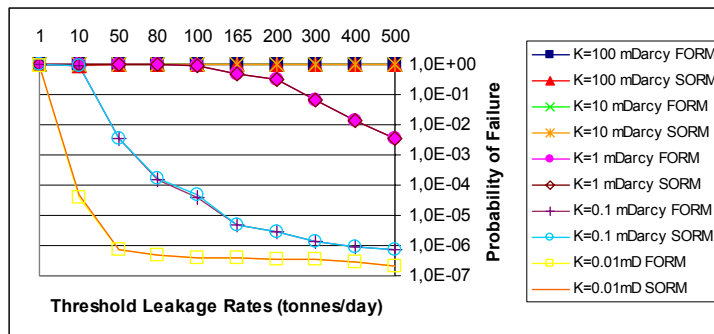


Figure 2: Probability of failure of a fault at different intrinsic permeability values with lognormal distribution at different threshold levels.

Additional valuable information to the failure probability and the parametric sensitivity factors is provided by the *importance factors*. Those were briefly explained in Section 2 and they indicate the relative importance of the uncertainty in each basic probabilistic variable. Figure 3 is an example that shows the change in importance factors with changing the threshold leakage rates along with the differential pressure across the fault and the dimensions of the fault (its width, length and depth) for the fault permeability case of $k=1$ mD. It is clear that in this case for the given mean fault permeability, the probabilistic outcome is sensitive to all the parameters for all threshold leakage rates, which implies that all parameters contribute equally to the uncertainty. We introduced in Equation (6) a term that accounts for the effect of coupling the hydrology and geomechanical processes, a permeability change factor which is an empirical relationship between the permeability and the change in differential pressure, after [14] in order to investigate the impact of pressure-induced changes in fault zone permeability. For the case with no coupling of hydromechanics the effect of other parameters being more pronounced relative to the differential pressure (Figure 3a) compared to the one with hydromechanical coupling (Figure 3b). In the latter the effects of the other parameters

(the dimensions including the permeability of the fault) are less than 30% whereas more than 70% is attributed to the sensitivity to the uncertainty in differential pressure. This implies that uncertainty in differential pressure is significant and more critical than the geometry of the fault. This result further suggests that increase of the fault permeability as a consequence of hydromechanical coupling would cause an increase in leakage rates and hence increasing the probability of failure. The results of the sensitivity analysis in this case are not intended to be general and can vary with the choice of problem configuration, prescribed probability distributions, and other pertinent factors. However, the methodology can be applicable to most cases of containment failure in CO₂ geological storage.

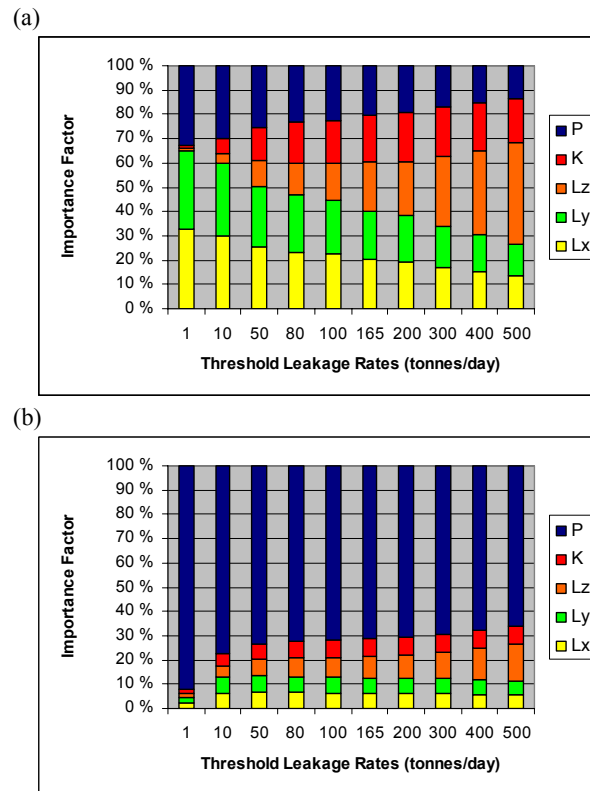


Figure 3: Importance factors of the parameters differential pressure, permeability and dimensions of the fault for mean fault permeability of 1 mDarcy case (a) With no permeability change factor and (b) with permeability change factor applied

6. Discussion and conclusion

Semi-analytical reliability methods FORM and SORM can generally provide probabilistic results that supplement or in some cases replace Monte Carlo (or similar directional simulation) methods. This study demonstrates application of FORM and SORM using the commercial software PROBAN [7] on an isolated description of vertical flow of CO₂ through a fault plane. We anticipate significant improvements in uncertainty analysis in general and in computational efficiency in particular when applying reliability methods to more complex CO₂ containment problems. FORM and SORM are potentially very attractive alternatives to the classical Monte Carlo simulation method when dealing with many independent CO₂ leakage events that have very small probability of occurrence, therefore requiring millions of Monte Carlo simulation function calls to converge. FORM and SORM were used to assess the probability that a given leakage from a fault exceeds a certain threshold level at a selected point in space and time in the solution domain and to provide the sensitivity of such a probabilistic event to the basic uncertainty in

the input variables. It is anticipated, however, that more complete testing of FORM and SORM results against other methods such as the Monte Carlo simulation will be performed.

The impact of the basic uncertainty in differential pressure and dimensions of the fault were identified. However, these parameter uncertainties are also dependent on the fault permeability which is important factor to consider in the probabilistic analysis of leakage from a fault. Potential rates of CO₂ flow along leakage pathways are difficult to constrain because of the unknown geometry and dimension of the potential leakage pathways [14]. However, this study demonstrated that the geometrical issues can be handled by considering the dimensions as probabilistic variables. Equation (6) can with reasonable assumptions provide an alternative for calculating flow rates along faults or fault zones that capture the complex flow pathways into a simplified model. This equation can be modified to account for the effect of coupling hydrological and geomechanical processes by introducing a permeability change factor which is a function of the differential pressure [14] and the effect of change in permeability on the probability of failure as a result of the coupling process can be investigated (future work). Over all the method of reliability analysis is proved to be applicable to CO₂ geological storage case and when leakage rates are constrained by natural analogues the failure probability would be more meaningful.

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